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Research Article

Anisotropic Elastic and Lattice Dynamical Properties of Cr_2AB MAX Phases Compounds

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Abstract

The structural, mechanical and lattice dynamical properties of the MAX Phase borides compounds *Cr_2AB (A= Al, P, Si)* have been investigated using the first principles calculations with the generalized gradient approximation (GGA) based on Density Functional Theory (DFT). The obtained negative formation energies of *Cr_2AB* indicate that these compounds are stable and could be synthesized. Some basic physical parameters such as lattice constants, elastic constants, bulk modulus, Shear modulus, Young's modulus, and Poison's ratio have been calculated. Ionic character has been found for *Cr_2AB* compounds. Also, *Cr_2AlB* is a brittle material while *Cr_2SiB* and *Cr_2PB* are ductile materials. In addition, the elastic anisotropy has been visualized in detail by plotting the directional dependence of linear compressibility, Poisson ratio, Young's and Shear moduli. Furthermore, electronic band structures and corresponding partial density of stated have been examined and it has been found that these compounds have metallic character. Moreover, the phonon dispersion curves as well as corresponding phonon partial density of states (PDOS) have been obtained. This study is the first investigation of the MAX Phase borides compounds *Cr_2AB (A= Al, P, Si)* and could lead to the future studies.

Keywords: MAX phases, borides, density functional theory, electronic properties, vibrational properties.

1. Introduction

Ionic, metallic and covalent bonding of the MAX phases with $M_{(n+1)}AX_n$ formula where n=1,2 and 3, provide unmatched properties [1,2]. The crystal structure of the MAX phases is hexagonal where M atom is a transition metal, A atom is an A group element, and X atom is Carbon and/or Nitrogen [2]. The MAX phases have good machinability properties, excellent electronic conductivity, thermal shock resistance, rather low weight, chemical stability and heat resistance due to having both metallic and ceramic properties [3]. As a result of these properties, the MAX phase could be used for applications such as wear and corrosion resistant coatings [4], superconducting materials [5] and nuclear industry [6].

MAX phases have three different atoms and the combination of these atoms lead to a vast number of possibilities. Until this time, the number of synthesized MAX phases is around 60 [7]. For these phases, the majority structure is 211 phase with *n*=1 and also, the most well established and the most examined materials are Ti_2AlC and Ti_3SiC_2 [8-12]. Recently, new materials and combinations from the MAX phase family have been focused in the literature. One of the most interesting and intriguing change is the replacement of Nitride or Carbide in X atom with Boron [13-15]. In this way, borides of MAX phases become an interesting study. But boron containing studies are not much in contrast to nitride and carbide containing studies in the literature. Therefore, *Cr_2AB* where A = Al, P, Si compounds have been considered in this study. Moreover, the outcomes have been compared with *Cr_2AC* where A = Al, P, Si and *Cr_2AlN* studies from the literature [3, 7-9, 11-14,16,17]. As known up to date, this is the first investigation of *Cr_2AB* compounds.

In this study, three *A* combinations for borides of MAX phases (*Cr_2AB* where A = Al, P, Si) compounds have been investigated using Ab-inito calculations. The calculation details have been presented in Section 2. The outcomes of the calculations have been detailed in Section 3 with three subsections. In Section 3.1, the *Cr_2AB* compounds have been examined for their structural and electronic properties. The mechanical properties have been studied in order to discuss the technological applications of these compounds in Section 3.2. The vibrational properties including phonon dispersion curves, phonon partial density of states (PDOS) and thermal properties have been presented in Section 3.3. A brief summary has been presented in Section 4.

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2. Computational Methods

The Vienna Ab initio Simulation Package (VASP) [18] has been used for DFT calculations. The projector augmented-wave (PAW) method [19, 20] has been used for electron-ion interaction with cut off energy of 550 eV. The generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) functional [21] has been chosen for the exchange and correlation terms in the electron-electron interaction. The Brillouin zone (BZ) sampling has been used for convergence tests. The converged results have been achieved with 16 x 16 x 4 k-point Gamma centered mesh [22].

The ground state geometries for Cr_2AB compounds have been found using the conjugate gradient algorithm. The stresses and Hellman-Feynman forces have been minimized with a force converge criteria less than 10^{-8} eV Å^{-1}. For the iterative solution of the Kohn-Sham equations, the energy tolerance is chosen less than 10^{-9} eV per unit cell. The Methfessel-Paxton method [23] in the order of 1 have been used for the all relaxations. In order to determine precise energy values, the tetrahedron method with Blöchl corrections [24] have been employed.

The strain-stress method implemented in VASP [18, 25] has been used to calculate the elastic constants. The calculated elastic constants have been employed to ELATE program [26] in order to get the anisotropic elastic properties. ELATE [26] is an open-source elastic tensor analysis software compiled from EIAM Code [27]. In addition, PHONOPY software [28] have been used to determine the phonon dispersion curves and phonon density of states and the density functional perturbation theory (DFPT) [29] implemented in VASP have been used to calculate the force constant matrices. Sufficient convergence with respect to the forces has been achieved for a 2 x 2 x 1 (32 atoms with an 8 x 8 x 4 kpoint mesh) supercell. The same kinetic energy cut off has been used for DFPT calculations.

3. Results and Discussion

3.1. Structural and Electronic Properties

The crystal structure of Cr_2AB (*A=Al, P, Si*) compounds is hexagonal structure with the space group $P6_3/mmc$ as shown in Figure 1. The Wyckoff positions of the *Cr* atom is 4f (1/3, 2/3, z), *A* atom is 2d (1/3, 2/3, 3/4), and *B* atom is 2a (0, 0, 0).

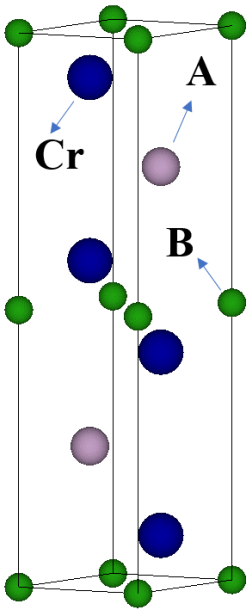


Figure 1. The crystal structure of Cr_2AB compounds

The optimized lattice parameters (a and c in Å), c/a ratio, z parameter of the Wyckoff positions, density (ρ in g/cm^3) and formation energy (ΔH_f in eV/atom) of the Cr_2AB compounds are listed in Table 1 and the results of the Cr_2AC and Cr_2AN studies from the literature are also listed to compare the calculated parameters. For Cr_2AlB compound, both Cr_2AlC and Cr_2AlN have been studied while only Cr_2PC and Cr_2SiC have been studied for comparison of Cr_2PB and Cr_2SiB in the literature. If the *X* atom changes from nitrogen to boron for Cr_2AlX, the compounds have larger lattice parameters as can be concluded from Table 1. Also, Cr_2PB and Cr_2SiB has higher lattice parameters than Cr_2PC and Cr_2SiC. In addition, the formation energy has been calculated using Equation 1 as given in Table 1. Negative formation energy indicates that these compounds are energetically stable and synthesizable.

$$E_{formation}^{Cr_2AB} = E_{Total}^{Cr_2AB} - 2E_{Solid}^{Cr} - E_{Solid}^{A} - E_{Solid}^{B} \quad (1)$$

Table 1. Lattice parameters (a and c in Å), c/a ratio, z parameter of the Wyckoff positions, density (ρ in g/cm^3 and formation energy (ΔH_f in eV/atom) of the *Cr_2AB* compounds

Compounds	Ref	*a*	*c*	*c/a*	*z*	*ρ*	*ΔH_f*
Cr_2AlB	Present	2.885	12.710	4.405	0.089	5.140	-0.108
	[13]	2.884	12.733	4.415	0.089		
	[14]	2.884	12.729			5.136	
Cr_2AlC	[3]	2.860	12.800			5.240	
	[16]	2.863	12.814			5.210	
Cr_2AlN	[7]	2.847	12.689		0.082		
	[13]	2.841	12.694	4.469	0.082		
	[17]	2.839	12.708		0.082		
Cr_2PB	Present	3.092	10.343	3.345	0.105	5.650	-0.268
Cr_2PC	[8]	2.947	10.948	3.715			
Cr_2SiB	Present	2.917	11.741	4.025	0.098	5.570	-0.263
Cr_2SiC	[9]	2.841	11.861	4.175	0.089	5.742	

The band structures for *Cr_2AB* compounds have been forecasted throughout the high symmetry points in the first Brillouin zone. Figure 2 and Figure 3 show the band structures and corresponding partial density of states (PDOS), respectively. In addition, these compounds have metallic characters as can be inferred from figures.

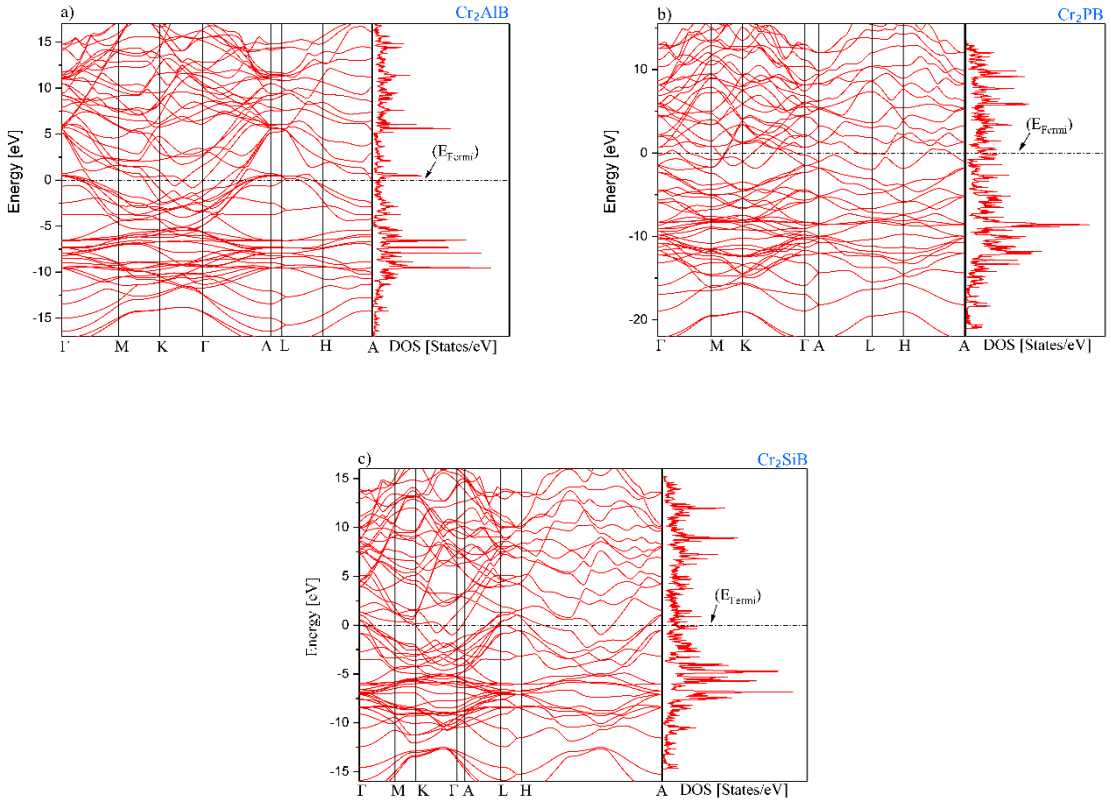


Figure 2. Band structure of (a) Cr_2AlB, (b) Cr_2PB and (c) Cr_2SiB compounds

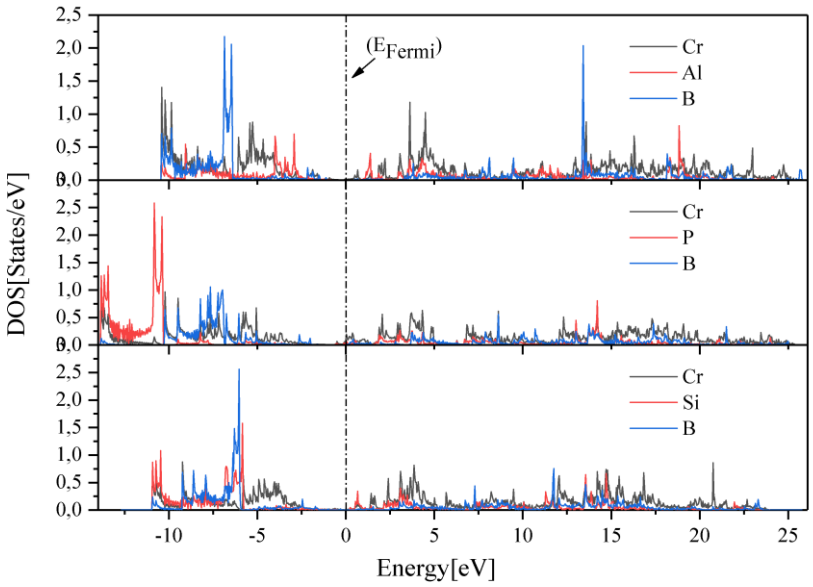


Figure 3. Partial density of states of Cr_2AB compounds

3.2. Mechanical Properties

The mechanical and dynamical behavior of a material could be determined using elastic constants (C_{ij}) which are also important for any technological applications. The material's hardness, stability and stiffness could be revealed from elastic constants which are C_{11}, C_{12}, C_{13}, C_{33}, and C_{44} for hexagonal structures. Table 2 lists the determined elastic constants for *Cr_2AB* compounds. The Born - Huang criteria [30] should be used to determine the mechanical stability of these compounds where the calculated constants satisfy these conditions. Therefore, all possible *Cr_2AB* crystal structures are mechanically stable as can be concluded from Table 2.

Table 2. Calculated elastic constants (Cij in GPa) for Cr2AB compounds

Compounds	Ref	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}
Cr_2AlB	present	296.84	83.92	127.33	295.81	106.46
	[13]	323.00	94.10	141.80	311.50	162.30
	[14]	298.78	81.86	129.78	289.62	157.37
Cr_2AlC	[13]	394.30	103.90	109.10	352.10	138.00
	[17]	369.00	77.00	102.00	355.00	143.00
	[11]	384.00	79.00	107.00	382.00	147.00
Cr_2AlN	[13]	253.40	50.00	90.90	320.50	76.00
	[17]	282.00	85.00	141.00	362.00	77.00
Cr_2PB	present	327.21	146.47	192.32	351.57	90.37
Cr_2PC	[8]	325.00	152.00	191.00	365.00	123.00
Cr_2SiB	present	313.52	126.01	179.31	348.80	93.75
Cr_2SiC	[12]	305.00	132.00	172.00	385.00	64.00
	[9]	337.00	138.00	178.00	440.00	64.00
	[8]	318.00	147.00	160.00	401.00	66.00

Bulk, shear and Young's moduli are used to determine a material's resistance to hydrostatic pressure, a material's response to shear stress and stiffness of a material, respectively. The Bulk (B) and Shear (G) moduli with the Voigt-Reuss-Hill (VRH) approximations [28] could be calculated using the elastic constants. If a strain uniformly applies to a crystal, the upper limit is Voigt bound while the lower limit is Reuss bound. Hill approximation given in Equation 2, is generally applied to obtain acceptable results.

$$B = (B_V + B_R)/2,\ G = (G_V + G_R)/2 \quad (2)$$

Here, V and R subscripts stand for Voigt and Reuss bounds, respectively. For each crystal structure, their own elastic constants are used to obtain the inclusive expressions of these bounds. Additionally, Equation 3 has been used to determine the Young's modulus (E) and Poisson's ratio (ν).

$$E = 9BG/(3B + G), \qquad \nu = (3B - 2G)/[2(3B + G)] \quad (3)$$

The values given in Table 3 have been obtained using Equation 2 and Equation 3. *Cr_2PB* has the highest bulk and Young's moduli while *Cr_2SiB* has the highest shear modulus. The bonding nature of the *Cr_2AB* compounds could be verified using the values of

Poisson's ratio (ν). The covalent bonding materials have ν value of about 0.1 while ν is around 0.25 for ionic materials [31]. *Cr_2AB* compounds have ionic bonding as can be inferred from Table 3. Also the B/G ratio provides the information about the ductility or brittleness character of a material as given in Table 3. *Cr_2AlB* has the B/G ratio lower than 1.75 that concluded brittleness of *Cr_2AlB* [15]. *Cr_2PB* and *Cr_2SiB* have the B/G ratio higher than 1.75 therefore these compounds are ductile. G/B ratio also called Pugh's modulus provide to find out the bonding nature of a material. For the dominantly covalent bonding materials, Pugh's modulus is around 1.1. If the material dominant bonding character is ionic, the Pugh's modulus is around 0.6 [31]. For the studied compounds, Pugh's moduli are around 0.6 which indicates dominant ionic bonding.

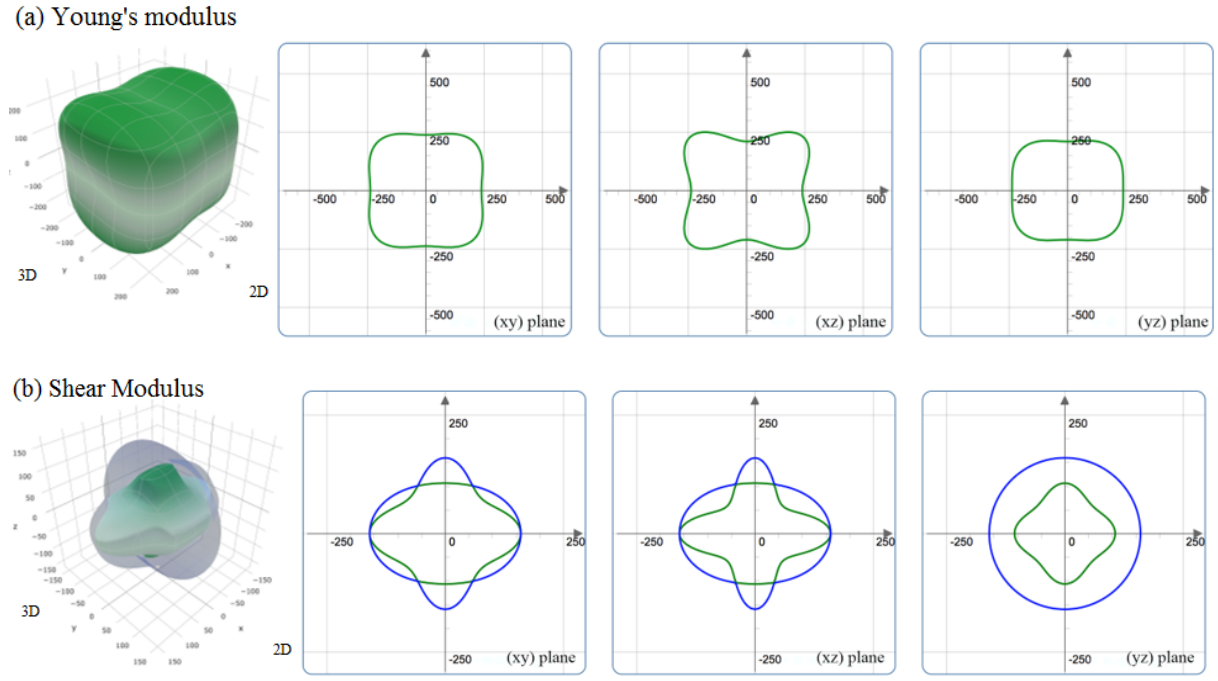
Table 3. Calculated bulk modulus (B, in GPa), Young's modulus (E in GPa), Shear Modulus (G, in GPa), Poisson's ratio (ν), B/G ratio, G/B ratio and Hardness (H_v, in GPa) for *Cr_2AB* compounds.

Materials	Ref	B	E	G	ν	B/G	G/B	H_v
Cr_2AlB	Present	173.64	287.44	117.41	0.22	1.48	0.68	18.24
	[13]	190.00	122.00	301.50				
	[14]	174.07	116.29	285.33	0.23			
Cr_2AlC	[13]	198.10	337.20	138.60				
	[3]	166.00	245.00	116.00	0.20			
Cr_2AlN	[13]	141.20	221.30	89.30				
Cr_2PB	Present	228.46	308.38	120.93	0.28	1.89	0.53	19.70
Cr_2PC	[8]	228.00		99.00				
Cr_2SiB	Present	214.04	306.40	121.45	0.261	1.76	0.57	25.92
Cr_2SiC	[12]	213.20	204.90	76.40	0.33			
	[9]	179.50	225.00	84.50	0.33			

Also, Chen et al. [32] developed the semi-empirical method based on Pugh's modulus ratio and it is given in Equation 4 that has been used to calculate the hardness of the compounds. The hardest compound among the studied compounds is *Cr_2SiB*.

$$H_V = 2(k^2G)^{0.585} - 3; (k = G/B) \quad (4)$$

The physical or mechanical properties such as dislocation dynamics, unusual phonon modes, anisotropic plastic deformation, precipitation, and etc. [33] are affected from the anisotropy of elasticity of a material. Moreover, formation of micro-cracks originated from the elastic anisotropy must be understood in order to improve the mechanical durability of a material in any application [34]. Therefore, elastic analysis of a material could be completed with the study of anisotropic elastic calculations. Here, ELATE code has been employed to visualize and calculate the directional dependence of the Young's modulus, linear compressibility, Shear modulus, and Poisson ratio shown in Figure 4. Young's modulus, shear modulus, Poisson's ratio and linear compressibility having distorted spherical shapes are anisotropic in all planes except the linear compressibility in xy plane. Also, the minimum points are shown with green curves while the maximum points are shown with blue curves for the studied parameters. In addition, Table 4 lists the maximum and minimum values of Young's modulus, shear modulus, Poisson's ratio and linear compressibility.



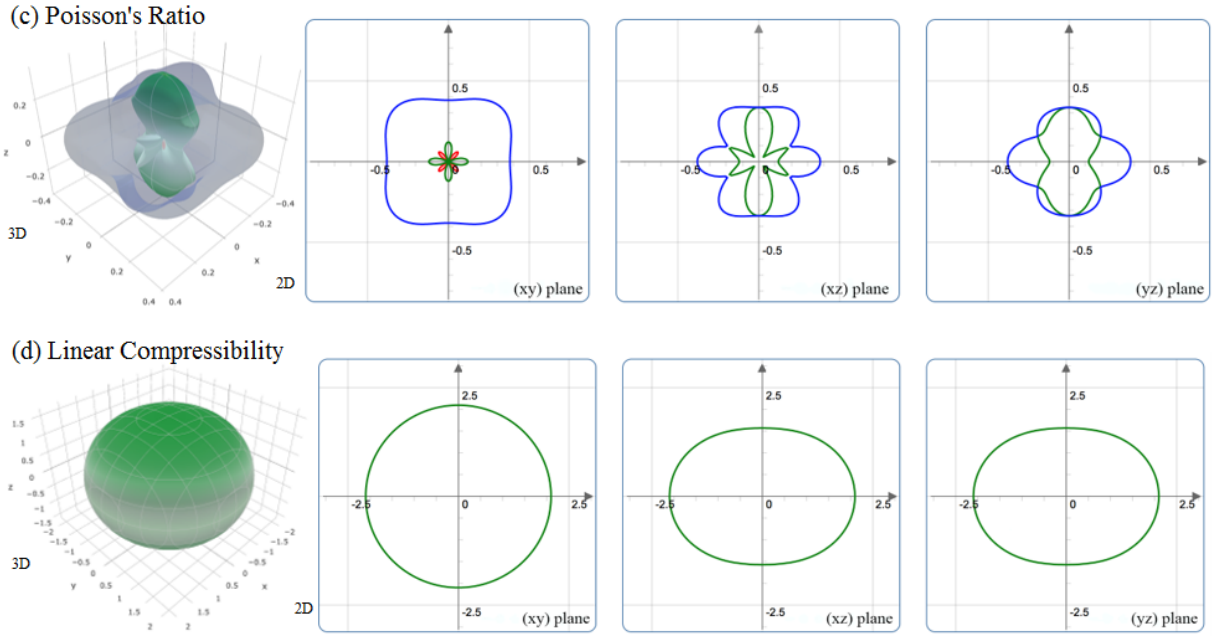


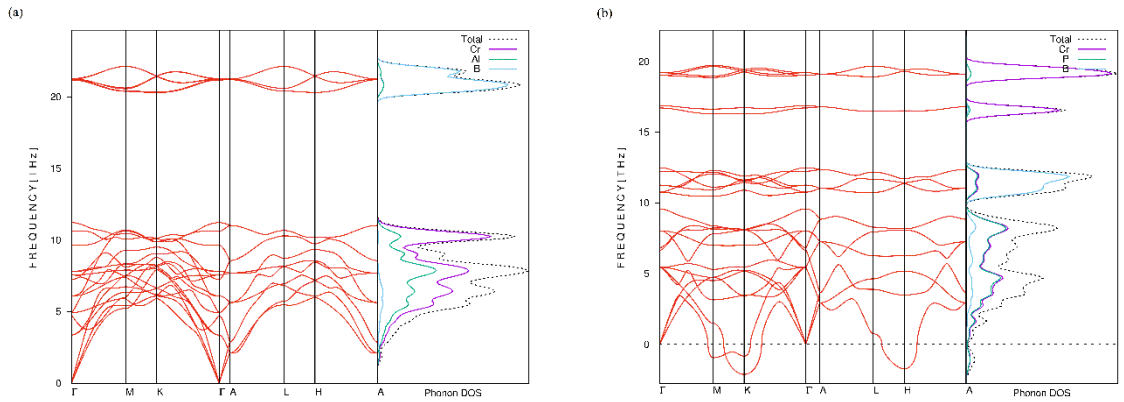
Figure 4. The calculated directional dependence of the mechanical properties; (a)Young's modulus, (b) Shear Modulus, (c) Poisson's ratio, and (d) linear compressibility for Cr_2AlB compounds

Table 4. Maximum and minimum values of Young's modulus (E_{min} and E_{max}, in GPa), linear compressibility (β_{min} and β_{max}, TPa^{-1}), Shear modulus (G_{min} and G_{max}, GPa) and Poisson's Ratio (ν_{min} and ν_{max}) for Cr_2AB compounds

Materials	Young Modulus		Linear Comp.		Shear Modulus		Poisson's Ratio	
	E_{min}	E_{max}	β_{min}	β_{max}	G_{min}	G_{max}	ν_{min}	ν_{max}
Cr_2AlB	210.70	336.00	1.57	2.10	82.55	159.91	-0.08	0.46
Cr_2PB	195.40	388.90	0.96	1.72	71.74	211.43	-0.23	0.67
Cr_2SiB	202.50	385.20	0.91	1.90	73.57	204.78	-0.23	0.63

3.2. Vibrational and Thermodynamic Properties

The dynamical stabilities of *Cr_2AB* compounds have been checked with the calculation of the phonon frequencies and phonon dispersion curves using the supercell approach with the linear response method. Figure 5 shows the obtained phonon dispersion curves and the corresponding phonon density of states (PDOS) for *Cr_2AB* compounds. There are 24 branches in the figures where 3 of them are acoustic and remaining are optic branches. There are no soft modes for *Cr_2AlB* and *Cr_2SiB* compounds while *Cr_2PB* compound has soft modes. Therefore, *Cr_2PB* is dynamically unstable. Moreover, this result is consistent with the electronic band structure where at the Fermi level, *Cr_2PB* has electrons as can be concluded from Figure 3.



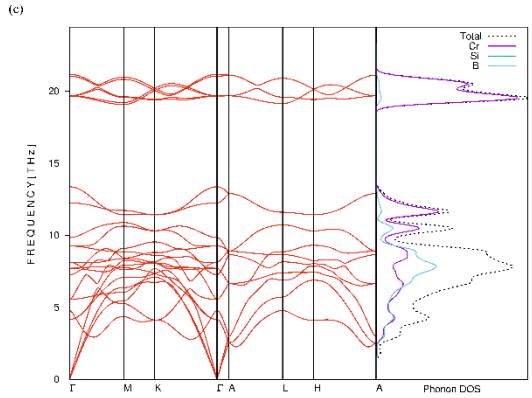


Figure 5. Phonon dispersion curves and PDOS for (a) Cr_2AlB, (b) Cr_2PB and (c) Cr_2SiB

The phonon information and the quasi-harmonic approximation have been used to determine the thermodynamic quantities, such as the Helmholtz free energy, enthalpy, entropy, and constant volume heat capacity (C_V) in 0 to 2000 K temperature range for *Cr_2AlB* and *Cr_2SiB* compounds. Figure 6a and Figure 6b show the free energy, enthalpy, entropy, and heat capacity as a function of temperature for *Cr_2AlB* and *Cr_2SiB*, respectively. *Cr_2PB* has not been given due to its dynamical unstability. Just as the temperature goes from 0 to 2000 K, the entropy enlarges while the free energy decreases. Also, the enthalpy increases almost linearly with the temperature after 300 K. Moreover, the heat capacity reaches a constant called Dulong-Petit limit for high temperatures higher than 700 K.

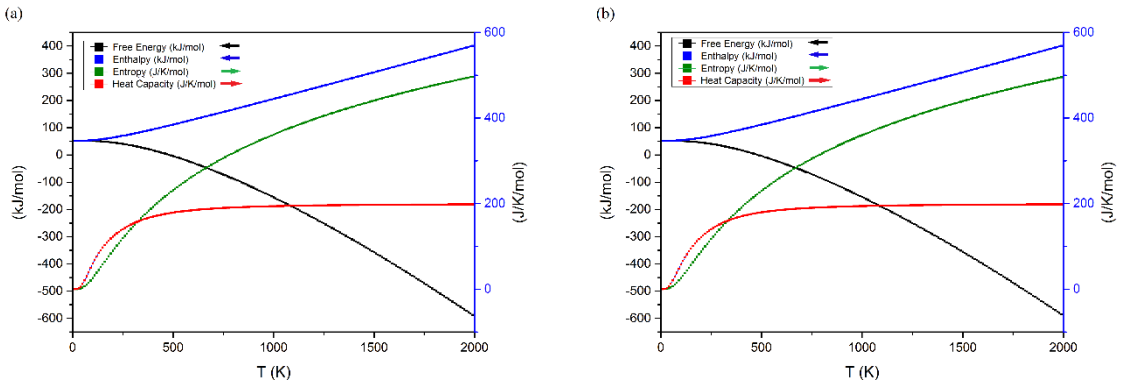


Figure 6. Free energy, enthalpy, entropy, and heat capacity as a function of temperature for (a) Cr_2AlB and (b) Cr_2SiB

4. Conclusion

The structural, mechanic, electronic, and dynamic properties of *Cr_2AB* compounds have been calculated using VASP. These compounds are energetically stable and synthesizable due to having negative formation energies. All materials have a metallic character as can be inferred from the obtained band structures. Furthermore, all materials are mechanically stable that have elastic constants satisfying Born-Huang stability criteria. Also, *Cr_2SiB* has the highest shear modulus in the studied compounds while the highest bulk and Young's moduli belong to *Cr_2PB*. All compounds have ionic bonding but *Cr_2AlB* is brittle and *Cr_2PB* and *Cr_2SiB* are ductile materials. In addition, *Cr_2SiB* is the hardest compound among the studied compounds. In the phonon dispersion curves, there are soft modes for *Cr_2PB* which is dynamically unstable material and the other materials have no soft modes that are dynamically stable materials. As a result, *Cr_2AB* phases can be taken into consideration for a candidate for the family of MAX phases. These calculations and analysis of the properties for hypothetical *Cr_2AB* phases could also be helpful in the future experimental and theoretical studies.

5. Acknowledgments

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